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To: Goma 6.0 Open-Source User Community

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Subject: Goma and SEACAS tutorial for new users (GT-001.9)

# MODEL PROCEDURE

This memo is the beginning of an extensive tutorial documentation designed to teach the details of using Goma to solve complex problems.

This particular tutorial is designed to give *the beginning user* practice in running a complete analysis using SEACAS and Goma, from the model definition to mesh generation to simulation to visualization. This particular tutorial is aimed at coating and related processing flow applications. However, it should be useful to a wider audience. To run through this tutorial you need a "tutorial" subdirectory. Hopefully what follows will enable the beginning user to get a feel for the capabilities, limitations, and proper procedure for running Goma, together with the pre- and post-processing capabilities in SEACAS, on two problems of relevance to continuous liquid film coatings. Eventually the contents of this tutorial will be included in the user documentation, but for now it should be used as a supplement.

First it is important for new users to put the code Goma into perspective. We highly recommend that you read the first three chapters of the Goma 6.0 user's manual as an introduction (goma.github.io). Goma 6.0 is currently considered a production code which solves simultaneously any combination of four branches of continuum mechanical equations: momentum transport in a fluid (e.g. the Navier-Stokes equations), momentum transport in a solid (e.g. the stress balance for an elastic solid), convective-diffusion transport of energy, and convective-diffusion transport of an arbitrary number of species. Auxiliary to these branches of mechanics, Goma also supports a host of related transport and definition equations. Examples include, but are not limited to, the voltage equation, viscoelastic constitutive equations, Reynolds lubrication equations, Reynolds film flow equations, and many more. Most limitations of Goma stem from the lack of boundary conditions for specialized situations and from the lack of material behavior. For this reason we have implemented a user-defined subroutine capability that allows for a wide range of customization and generalization.

Perhaps the most unique feature of Goma is that all nonlinear algebraic equations that result from the finite element discretization of the continuum differential equations are solved simultaneously (including all boundary conditions and constraints) with Newton's method. In other words, all solution

sensitivity is embodied in a single matrix called a Jacobian matrix. The availability of this matrix will be exploited in our stability/frequency response and optimization wrappers in later releases.

# **DESCRIPTION OF THE SOFTWARE:**

The two main "distributions" of software required for ease of analysis using Goma are:

- *Goma* 6.0 is a finite element program which excels in analyses of multiphysical processes, particularly those involving the major branches of mechanics (viz. fluid/solid mechanics, energy transport and chemical species transport). *Goma* is based on a full-Newton-coupled algorithm which allows for simultaneous solution of the governing principles, making the code ideally suited for problems involving closely coupled bulk mechanics and interfacial phenomena. Example applications include, but are not limited to, coating and polymer processing flows, super-alloy processing, welding/soldering, electrochemical processes, and solid-network or solution film drying. This document serves as a user's guide and reference.
- SEACAS: Sandia-developed Engineering Analysis Code Access System (SEACAS) a modular system based upon a common binary data file format called EXODUS II which includes the mesh description and the time planes of the computed results. Most existing Sandia mechanics codes, including those mentioned herein, and all new Sandia-developed mechanics codes employ this database. The SEACAS system consists of pre- and post-processing codes, translation codes, support libraries, and scripts all designed to ease engineering application of Sandia-developed analysis codes. The system also includes some previously released finite element software for solid, fluid, and thermal analysis.

Additionally, extensive documentation exists on several forms, including a comprehensive user-manual, designed as a reference manual, an advanced capabilities manual for additional and unique design-toanalysis capabilities for linear stability, augmenting conditions and automated continuation, thin-shell equation manual and tutorial, additional usage tutorials and tech memo. This suite of documentation can be obtained from Sandia. *We should also mention that while mesh generation and post-processing visualization tools are available in SEACAS, they are very dated and not recommended (with the postprocessing tool "blot" being the exception). We recommend the users acquire Paraview (opensource, www.paraview.org) or Ensight for visualization, and Cubit/Trellis (www.csimsoft.com) for mesh* generation.

This tutorial will focus on the first two software distributions and is arranged as follows:

- 1. Introduction to the finite element database (i.e., file) ExodusII. Exodus libraries and translators exotxt, txtexo, ncdump, ncgen, etc.
- 2. Tools for generating, manipulating, and interrogating meshes and mesh data: CUBIT, GROPE, ALGEBRA, etc.
- 3. APREPRO: An algebraic preprocessor for parameterizing finite element analysis (or any analysis for that matter).

- 4. BLOT: A post-processing tool for ExodusII databases.
- 5. Introduction to Goma capabilities with respect to coating, related processing flows, and drying.
- 6. Tutorial problem: Knife coating flow with Goma
- 7. Sample tutorial problem: volume shrinkage and substrate curl.
- 8. APPENDIX A: FASTQ, GJOIN, GEN3D

# <u>1. EXODUS II</u>

EXODUS II is a library of routines that can be used to write a finite element database file (i.e. an Application Programming Interface, or API). The file format is binary and indirect access, but adheres to the IEEE XDR standard of binary, which allows the files to be freely transferred from machine to machine. EXODUS II employs a public domain database library, netCDF, to handle the low-level data storage. In fact, it is the netCDF library that provides machine independency as it stores data in eXternal Data Representation (XDR) format. Because EXODUS II files are actually netCDF files, an application program can access data via the EXODUS II API, the netCDF API, or XDR function calls directly.

Several tools exist in the SEACAS library of tools for manipulating and viewing an EXODUS II file.

- exotxt converts EXODUS II files into an ASCII text version for viewing.
- txtexo converts the ASCII text version back to an EXODUS II file
- ncdump converts an EXODUS II file to a netCDF text file for viewing or other purposes
- ncgen converts a netCDF text file back to a netCDF file or EXODUS II file.

Several things should be noted here. It is common practice to name your EXODUS II files with a ".exoII" extension, like "slot\_coating.exoII". Often times you will see files hanging around that have ".exo" and ".gen" extensions (or more abreviated ".e" and ".g" extensions). The ".gen" extension often times means that the file is in "Genesis" format, which is an EXODUS II file without the solution fields from the simulation, i.e., the file contains nodal coordinates, connectivity, and boundary element and nodal set information only.

## <u>EXODUS II TUTORIAL</u>

- 1) Change directories into the "tutorial" directory (this location will depend on the course you are taking and how you installed your software).
- You will notice a series of files with various extensions. One such file is the in.exoII file. Issue the following commands: ncdump in.exoII > dum.txt more dum.txt

You will notice that this file has a variety of finite element type information, like number of nodes per element, number of elements, etc.:

```
netcdf in {
dimensions:
        len string = 33 ;
        len line = 81;
        four = 4;
        time step = UNLIMITED ; // (0 currently)
        num dim = 2;
        num nodes = 25 ;
        num elem = 4;
        num el blk = 2 ;
        num node sets = 4 ;
        num_side_sets = 5 ;
        num el in blk1 = 2 ;
        num nod per el1 = 9 ;
        num el in blk2 = 2;
        num_nod_per_el2 = 9 ;
        num nod ns1 = 5;
        num_nod ns2 = 5 ;
        num nod ns3 = 5 ;
        num nod ns4 = 5;
        num side ss1 = 2 ;
        num df ss1 = 6;
        num side ss2 = 2;
        num df ss2 = 6;
        num side ss3 = 4;
        num df ss3 = 12;
        num side ss4 = 2;
        num df ss4 = 6;
        num side ss5 = 2;
        num df ss5 = 6;
        num qa rec = 1;
variables:
        float time whole(time step) ;
        long eb status(num el blk) ;
```

• • • •

This file is clearly a finite element database. You will notice a connectivity array, nodal coordinates, etc.

3) Next issue the command

```
ncdump in.gen
```

You will notice the statement:

ncdump: in.gen: NetCDF: Unknown file format

To summarize this section, these tools are usually needed when a user/developer is trying to understand in more detail how Goma is interacting and reading/writing these databases, or when a user wants to extract text-form information from the mesh or data for analysis. In general this is rare.

# 2. GROPE, ALGEBRA (and FASTO)

There are many tools in the SEACAS distribution which can be used to generate meshes, manipulate meshes, and interrogate ExodusII files. Until recently we including SEACAS mesh generator FASTQ

in our training, but now it is so obsolete compared to tools like CUBIT that we have relegated that training module to Appendix A. That said, not everyone has CUBIT, as it is not free, so we felt we had better keep it. Please consult Appendix A to learn how to use FASTQ/GJOIN/GEN3D. We will also run FASTQ in other parts of this tutorial, as needed, and even demonstrate a FASTQ translator in CUBIT.

Some other tools which are worthy of quick mention are:

- GROPE can be used to extract and manipulate EXODUS II files. Often times you want to extract a value of a variable at a specific location (node) or along a specific side (side set), like pressure along a permeable substrate, for instance. GROPE can be used to do this. The documentation is fairly complete and easy to understand.
- ALGEBRA is similar to GROPE but allows you to define other variables based on your current nodal variable set. For instance, you may want to plot only dimensional quantities, even though your EXODUS file contains nondimensional ones. In ALGEBRA, you can define dimensional versions and output a new EXODUS file with those versions to be plotted by BLOT. Again, the documentation for ALGEBRA is complete and easy to understand

# <u>3. CUBIT</u>

CUBIT is a two- and three-dimensional finite element mesh generation toolkit. The CUBIT Development Team at Sandia National Laboratories has developed and maintains this toolkit for the most part. But since 2005 or thereabouts CUBIT is being distributed with commercial licenses for a fee. Toolkit and licensing information for CUBIT can be found at their website: http://cubit.sandia.gov and also at www.csimsoft.com

The CUBIT Development Team hosts biannual training classes (Introductory and Advanced) so we will not attempt to duplicate these sessions. Our purpose here is to provide rudimentary skills to carry a user through the required mesh development stage necessary for Goma training.

CUBIT can be run in three modes - interactive with a graphical user interface (GUI), interactive via command line, and batch mode. This brief introduction to CUBIT will use the interactive command line method of data entry/mesh development. We will duplicate mesh development for the simple 2D box problem.

The primary steps in creating a finite element mesh with CUBIT are geometry creation, interval and scheme specification, meshing the geometry, assigning boundary flags and exporting the mesh. These are detailed below. Note the following text format used here: commands entered by the user are in **bold** print while responses/echoes from CUBIT are in **bold italics** print.

### 1. Geometry Creation:

The topological entities in CUBIT consist of vertices, curves, surfaces, volumes and bodies, each with a corresponding dimension to it. Each topological entity is bounded by one or more entity of lower dimension. A body is not required for a complete topological model but is a convenient mechanism for grouping volumes. Geometries can be created in CUBIT by one of three primary methods: built up from

a set of geometry primitives, such as spheres or bricks; defined from the "bottom up" by creating vertices, then curves, etc.; or finally by importing an ACIS ".sat" file (which forms the solid model portion of CUBIT).

A simple box is meshed by the following commands using the geometry primitives. As CUBIT is fully 3D by default, a simplistic approach is used to limit graphical displays to two dimensions, i.e., change the display mode.

```
graphics mode hiddenline
```

```
To create a 1-by-1 box
```

create brick x 1 y 1
brick body 1 successfully created
Journaled Command: create brick x 1 y 1

This gives us the basic geometry, a set of vertices with connecting line segments defining an enclosed region. In CUBIT, this entity is a *volume*. We can check the numbering of the created entities by using various label options. Look at vertices, curves and volumes, turning off the labeling on the previous entity before proceeding to the next.

```
label vertex
label off
label curve
label off
label volume
graphics mode wireframe
```

The return to "wireframe" mode allows the user to view the volume number placed at the centroid of the body, a value that cannot be seen when "hiddenline" mode obscures the third dimension.

```
label off
graphics mode hiddenline
label surface
display
```

This final display shows the portion of the body we will mesh, i.e., surface 1.

### 2. Intervals and Scheme:

Element size can be controlled by specifying the mesh density for a particular entity; in this case, we will use the surface. Meshing scheme is left to default; CUBIT has a set of algorithms that use topological and geometry data to select the best meshing tool.

```
surface 1 size .5
Journaled Command: surface 1 size .5
```

#### 3. Meshing:

This is an extremely simplistic mesh so it does not illustrate the capabilities or the options present in CUBIT. After specifying the parameters and option in step 2, meshing is carried out by specifying a list of entities to mesh; as above, we use the surface of the volume.

mesh surface 1
Matching intervals successful.
Meshing Surface 1 (Surface 1)
Generated 4 elements for Surface 1 (Surface 1).
Surface 1 (surface 1) meshing completed using scheme: map
Journaled Command: mesh surface 1

The alternate "bottom up" method to reach the same stage can be executed with the following commands; these are listed only for illustration and comparison (unless you wish to investigate CUBIT further).

```
create vertex 0 0
Creation of Vertex 1 (Vertex 1) Successful.
Journaled Command: create vertex 0 0
create vertex 1 0
Creation of Vertex 2 (Vertex 2) Successful.
Journaled Command: create vertex 1 0
create vertex 1 1
Creation of Vertex 3 (Vertex 3) Successful.
Journaled Command: create vertex 1 1
create vertex 0 1
Creation of Vertex 4 (Vertex 4) Successful.
Journaled Command: create vertex 0 1
create curve 1 2
Creation of Curve 1 (Curve 1) Successful.
Journaled Command: create curve 1 2
create curve 2 3
Creation of Curve 2 (Curve 2) Successful.
Journaled Command: create curve 2 3
create curve 3 4
Creation of Curve 3 (Curve 3) Successful.
Journaled Command: create curve 3 4
create curve 4 1
Creation of Curve 4 (Curve 4) Successful.
Journaled Command: create curve 4 1
create surface 1 2 3 4
Creation of Surface 1 (Surface 1) Successful.
This is sheet body 1 (Body 1)
Journaled Command: create surface 1 2 3 4
```

surface 1 size .5
Journaled Command: surface 1 size .5
mesh surface 1
Matching intervals successful.
Meshing Surface 1 (Surface 1)
Generated 4 elements for Surface 1 (Surface 1).
Surface 1 (surface 1) meshing completed using scheme: map
Journaled Command: mesh surface 1

#### 4. Boundary Flags:

Sandia's EXODUS II format groups mesh information for elements and collections of nodes and element sides. These collections are termed Element Blocks, Node Sets and Side Sets, respectively. These are referenced in an analysis code by calling out a designation (i.e., an ID) assigned to these collections by the mesh generation software.

```
block 1 surface 1
Assigning Surface 1 to Element Block 1.
Journaled Command: block 1 surface 1
block 1 element type quad4
Journaled Command: block 1 element type quad4
nodeset 1 curve 1
Journaled Command: nodeset 1 curve 1
nodeset 2 curve 2
Journaled Command: nodeset 2 curve 2
nodeset 3 curve 3
Journaled Command: nodeset 3 curve 3
nodeset 4 curve 4
Journaled Command: nodeset 4 curve 4
sideset 1 curve 1
Journaled Command: sideset 1 curve 1
sideset 2 curve 2
Journaled Command: sideset 2 curve 2
sideset 3 curve 3
Journaled Command: sideset 3 curve 3
sideset 4 curve 4
Journaled Command: sideset 4 curve 4
```

#### 5. Export Mesh:

Setup and creation of the mesh has been completed; all that remains is to save the mesh data into an appropriately named file. (Note, the filename must be in single quotes.)

export genesis 'box.exoII' overwrite

```
File box.exoII will be written with the following version of EXODUS II:
API version: 3.220000
DB version: 2.050000
Preparing genesis mesh data ...done
Preparing genesis side set data . .1.2.3.4. done
Initializing genesis file...done
Writing coordinates....done
```

Writing element blocks...1...done Writing nodesets...1.2.3.4...done Writing sidesets...1.2.3.4...done Writing global order map...done Writing global element order map...done Writing global nodal order map...done Executive Genesis summary: number dimensions = 2 number nodes = 9 number elements = 4 number element blocks = 1 number NodeSets = 4 = 4 number SideSets Detailed Genesis summary: ----- Element Block Information ------Block 1 contains 4 exported 2D element(s) of type QUAD4. *Owned Entities:* \_\_\_\_\_Name\_\_\_\_\_Type\_\_\_\_Id Mesh\_Elements Surface 1 Surface 1 4 ----- NodeSet Information ------NodeSet 1: contains 3 nodes. Owned Entities: Name\_\_\_\_\_Id Mesh\_Elements 1 *Curve 1 Curve* 3 NodeSet 2: contains 3 nodes. Owned Entities: Name\_\_\_\_\_Type\_\_\_\_Id Mesh\_Elements Curve 2 Curve 2 3 2 3 NodeSet 3: contains 3 nodes. *Owned Entities:* \_\_Name\_\_\_\_ Type\_\_\_\_ \_\_\_\_\_Id Mesh\_Elements *Curve 3 Curve* 3 3 NodeSet 4: contains 3 nodes. Owned Entities: \_Name\_\_\_\_\_ Type\_\_\_\_Id Mesh\_Elements *Curve 4 Curve* ----- SideSet Information ------SideSet 1 contains 2 exported element sides. Owned Entities: \_\_\_\_Id Mesh\_Elements Sense Name \_\_\_\_\_Type\_\_\_\_ 1 2 *Curve 1 Curve* A11 SideSet 2 contains 2 exported element sides. Owned Entities:

\_\_\_\_Name\_\_\_\_ Type\_\_\_\_Id Mesh\_Elements Sense

Curve 2 Curve 2 2 A11 SideSet 3 contains 2 exported element sides. Owned Entities: Id Mesh Elements Sense Name Type 3 2 Curve 3 Curve A11 SideSet 4 contains 2 exported element sides. Owned Entities: \_Name\_\_\_\_\_ Type\_\_\_\_Id Mesh\_Elements Sense Curve 4 Curve 4 2 A11 Finished writing box.exoII

Removed 0 temporary NodeSets.

Journaled Command: export genesis "box.exoII"

Thus are the basic steps followed for a typical problem. If you want to iterate on the mesh, the current mesh can be eliminated via

```
delete mesh
...deleting 4 faces and 16 EdgeUses from database...
...deleting 12 edges from database...
...deleting 9 nodes from database...
Journaled Command: delete mesh
```

A new mesh density can be selected surface 1 size .2

or intervals can be specified along particular curves

```
surface 1 size .2
Journaled Command: surface 1 size .2
curve 1 interval 7
Journaled Command: curve 1 interval 7
curve 2 interval 10
Journaled Command: curve 2 interval 10
curve 2 scheme bias factor 1.2 start vertex 2
Journaled Command: curve 2 scheme bias factor 1.2 start vertex 2
surface 1 scheme pave
Journaled Command: surface 1 scheme pave
mesh surface 1
Matching intervals successful.
Meshing Surface 1 (Surface 1)
Paver grid cell factor changed to 5.2 for surface 1.
. . . . . . . . . .
Cleaning up paved mesh ..
```

Smoothing Surface Mesh... Generated 45 elements for Surface 1 (Surface 1). Surface 1 (surface 1) meshing completed using scheme: pave Journaled Command: mesh surface 1

Of course CUBIT is a very sophisticated solid-model/meshing package and we highly recommend their tutorials and their courses, which are very valuable.

# 4. APREPRO

APREPRO ("A PRE-PROcessor") is a tool that can be used to parameterize problems in terms of more familiar quantities. Basically, it is a text processor which allows the user to evaluate expressions and define variables according to a prescribed syntax. The output is also a text file which has all prescribed APREPRO syntax removed. Clearly, we can use this tool to generate input files (or "decks") for CUBIT and Goma. In this section we will give one brief example of how APREPRO can be used to parameterize a coating problem in terms of more familiar quantities, but we highly encourage you to read the manual insert in your documentation and study the tutorial examples below to get a feel for the extent of its capabilities.

### <u>APREPRO TUTORIAL</u>

Suppose we wanted to parameterize a two-layer slide coating flow in terms of quantities like inlet flow rate (or final film thickness), slide inclination angle, web angle with vertical, coating nip, slide length, etc. Goma and CUBIT require hard numbers to be input for geometry description (i.e. points and lines) and velocity boundary conditions. One of APREPRO's many useful features is that it can be used to evaluate simple arithmetic expressions and substitute the results where appropriate. The basic syntax is that any expression in curly braces "{}" is evaluated and the result is substituted upon output. This example illustrates the concept (please read the APREPRO manual for other more extensive features).

### SLIDE COATING DEFINITION FILE (FILE Defs)

```
$ Thermo-Physical Properties (all units mks)
$
$ viscosity
                                        \{visc1 = 0.01\}
                                        \{visc2 = 0.01\}
$
$ density
                                        \{densi1 = 1.e3\}
                                        \{densi2 = 1.e3\}
Ś
$ surface tension
                                        \{st1 = 0.07\}
                                        {st2
                                               = 0.07
$
$ gravity
                                        \{qrav = 9.8\}
$
$ OPERATING CONDITIONS
$ final thickness layer 1
                                         {finth1
                                                    = 45.e-6
                                         {finth2
                                                  = 45.e-6
$ final thickness layer 2
$ webspeed
                                         \{websp = 1.\}
                                             = websp*finth1}
$ flowrate layer 1
                                         {q1
$ flowrate layer 2
                                         {q2
                                                = websp*finth2}
$ slide angle with horizontal
                                        \{alpha = PI/10.\}
$ angle of web and gravity vector {beta = 0.}
$
```

```
$
   CALCULATION OF FILM THICKNESSES
$
    (NB! DENSITIES AND VISC OF BOTH LAYERS ARE THE SAME FOR NOW!)
$
$
   {cosab = cos(PI/2-alpha+beta)} {denom = densi1*grav*abs(cosab)/visc1}
$
   \{q1a = (q1+q2)/denom\}
$
  \{\text{thisl1} = (3*q1a)**(1./3.)\}
$
   \{thisl2 = 0.\}
$
$ Thin out initial guess a little more
$ slide film thickness
                                          {h1 = thisl1+thisl2}
$ web film thickness
                                          {h2 = (finth1+finth2)}
$ slide length
                                          \{S = 7.0 * h1\}
$ web length from top of slide
                                          \{W = 3.0*h1\}
$ coating nip (die face and web)
                                          \{G = 0.4 * h1\}
$ MESH PARAMETERS
Ś
${no elem along slide = 17}
${no elem along slide1 = 7}
\{no elem layer 1 = 3\}
\{no elem layer 2 = 3\}
${no elem across film = no elem layer 1 + no elem layer 2}
${no elem across gap = 5}
${no elem along web = 12}
```

When this tutorial problem was created, we did not use CUBIT to generate mesh. Instead, we employed FASTQ, a mesh generation program included in SEACAS distribution. As of this time, we have not updated the tutorial to use a CUBIT journal file for this slide-coater problem. So the syntax below is that for FASTQ. However, we can run this file through the CUBIT translator for FASTQ. One could use these same parameter definitions in a CUBIT journal file, of course.

```
FASTQ (CUBIT) INPUT FILE (slide.fas)
```

{include(Defs) }

```
$$$$This section begins the FASTQ input deck section$$$
Point 1 \{x1=G\} \{y1=-S*sin(alpha)\}
Point 2
              {x2=G+S*cos(alpha)}
                                       {y2=0}
Point 3
              x3=x2-h1*\cos(PI/2-alpha)
                                               {y3=y2+h1*sin(PI/2-alpha)}
$$NB the factor of 2 here is to make the initial guess better
              x4=G {y4=y1+h1/sin(PI/2-alpha)/2}
Point 4
Point 5
              {x5=h2} {y5=G+y4}
Point 555
             {x4+(x4+x5)/3.} {(y4+y5)/2.}
Point
       8
               \{x8=0\} \{y8=-S*sin(alpha)+G\}
             {x6=h2} {y6=W+y8}
Point 6
Point 7
              \{x7=0\} \{y7=W+y8\}
Point 9
               \{x9=0\} \{y9=y5\}
Point 20
               \{x20=(x2+x3)/2\} \{y20=(y2+y3)/2\}
Point 21
               {x21=x1}
                              \{y21=(y1+y4)/2\}
              \{x22=(x8+x4)/2\} \{y22=(y8+y4)/2\}
Point 22
       23 {x23=(x5+x9)/2} {y23=(y5+y9)/2}
24 {x24=(x6+x7)/2} {y24=(y6+y7)/2}
Point 23
Point
```

 ${y30=-S*2*sin(alpha)/3}$ Point 30  $\{x30=G+S*\cos(alpha)/3\}$ Point 32  $x32=G+S*\cos(alpha)/3-h1*\cos(PI/2-alpha)$ {y32=y30+h1\*sin(PI/2-alpha)/2}  $\{x31=(x32+x30)/2\}$  ${y31=(y32+y30)/2}$ Point 31 \$ Kramers rule for the solution of two equations and two unknowns is needed for the input of the line segments to salsa. \$ \$ 2 30 0 Line 1 STR {no elem along slide1} 1. 100 30 1 0 {no elem along slide} 0.95 Line STR Line 2 STR 2 3 0 {no elem across film} 1.0 Line 3 STR 3 32 0 {no elem along slide1} 1.0 Line 300 STR 32 4 0 {no elem along slide} 0.95 Line 4 5 4 555 . 9 CIRC {2\*no elem across gap} 4 5 0 \$\$Line 4 STR {no\_elem\_across\_gap} 1.0 5 5 6 0 {no elem\_along\_web} Line STR 1.2 Line 6 STR 6 7 0 {no elem across film} 1.0 7 7 8 0 Line STR {no elem along\_web+no\_elem\_across\_gap} 1.0 1 0 Line 8 STR 8 {no elem across gap} 1.0 Line 10 4 1 0 {no elem across film} STR 1.0 Line 11 STR 4 8 0 {no elem across film} 1.0 5 9 0 Line 12 STR {no elem across film} 1.0 Line 13 STR 8 9 0 {no elem across gap} 1.0 Line 14 9 7 0 {no elem along web} 1.2 STR 20 20 31 0 Line STR {no\_elem\_along\_slide1} 1.0 Line 200 STR 31 21 0 {no elem along slide} .95 22 0 Line 21 STR 21 {no elem across gap} 1.0 Line 22 STR 22 23 0 {no elem across gap} 1.0 0 Line 23 STR 23 24 {no elem along web} 1.2 Line 30 STR 2 20 0 {no elem layer 1} 1.0 Line 31 STR 20 3 0 {no elem layer 2} 1.0 32 24 7 0 Line {no elem layer 1} 1.0 STR {no elem layer 2} Line 33 STR 24 6 0 1.0 Line 34 1 21 0 {no elem layer 1} 1.0 STR Line 35 STR 21 4 0 {no\_elem\_layer\_2} 1.0 23 0 Line 36 STR 9 1.0 {no elem layer 1} 0 Line 37 STR 23 5 {no elem layer 2} 1.0

Note that the **Defs** file defines all sorts of well-known quantities, like thermophysical properties and slide coating geometry. Of course all of this is needed to prescribe the initial geometry that must be meshed up. So these quantities are then manipulated into film thicknesses, flow rates and eventually into point and line locations, however this is done in the **slide.fas** file in which file **Defs** is included. Look at each file to get a feel of how the **slide.fas** depends on **Defs**. The geometry description of the FASTQ input file starts below these definitions. In this case, we include the **Defs** file in the FASTQ input file. CUBIT, when this fastq input file is read in and translated automatically runs APREPRO. You can also run APREPRO before being read by CUBIT (FASTQ). That is, as part of this tutorial, issue the command

aprepro slide.fas dum.fas

Now look at dum.fas with "more dum.fas" and you'll see that the point and line commands have been evaluated and dum.fas is ready to be read into fastq. To automatically send these definition files "Defs" and "slide.fast" through this step without execution of APREPRO secperately, just run CUBIT with an import of slide.fas, which in turn includes the Defs file:

```
cubit
```

From the command line window:

CUBIT> import fastq `slide.fas'

or you can import the aprepro'd file:

CUBIT. import fastq `dum.fas'

That is, CUBIT automatically processes APREPRO syntax. Most of the tools in SEACAS which take or read in text input files support a "-a" option, which automatically runs the text input file through APREPRO before reading the file. FASTQ and Goma are two such tools, as is demonstrated here and below.

# 5. BLOT - A postprocessor

The BLOT program can be used to visualize an EXODUS II file by displaying the mesh and vector/contour plots of various quantities. It even allows for time history plots of quantities from particular points and some simple x-y plots from slices in the domain. It supports several device drivers, including X-windows (the default and what you will be looking at on your screen) and postscript (for obtaining hard copies). *BLOT is NOT for high-end, high-quality graphics, and some have said that it will become obsolete by 1995. Well, here we are in 2015 and BLOT is used extensively at Sandia, for no other reason than it is a quick-and-dirty visualizer that takes no memory, no start-up time and is expedient.* 

Basically BLOT is arranged in a multilayered structure, but its accompanying documentation and online help facility are not as good. At the upper-most level (called BLOT>) the user has several choices, including log, for saving a journal file, cmdfile, for reading from a previously saved journal file, detour, a multidimensional vector and contouring package, tplot, for time history plots, and splot, for spatial X-Y plots. You will mostly use detour and hence it is the only subpackage covered in this tutorial. It should be mentioned that BLOT does not take advantage of hardware graphics cards (i.e., for 3D rotation and volume rendering). However, it is an extremely fast graphics package that is more than adequate for all 2D problems and most 3D problems. This tutorial is designed to teach you some of the basic necessities.

# BLOT TUTORIAL

From the same "tutorial" subdirectory do an "1s" to list the files and choose an "\*.exoII" file to visualize. Let's choose the 3ddie.exoII file generated earlier because it is 3D and can be used to demonstrate how to do rotations.

1. To start BLOT with this file

#### blot 3ddie.exoII

You will note if you forget the exoII file name or just type "blot" you will get a help page advising you of all of your options.

2. Anyway, starting up BLOT results in a popped X-window on your screen. Often times it is nice to re-position that window so you have a clear view of both your command window and the graphics window. Now with blot you will see the following prompt:

BLOT>

Your options here are several, but the ones we will demonstrate here are log, cmdfile, and detour. Type "log" to save a journal file of this session.

BLOT>log

We will use this log file to record all of our BLOT commands and re-execute them in this tutorial. Type "detour" to enter the contouring and vectoring subroutine:

BLOT>det\*our

Note that you need only type "det"

3. You have many options here, but the first is to see what variables you have available to you for plotting. You can do this one of two ways. When you first entered BLOT you noticed just below the banner page it listed the nodal variables available. Another way is to issue the command:

```
DETOUR> list names
```

```
which results in

Variables Names:

History:

Global:

Nodal: VX VY

VZ P

PRESSURE

RMX

RMY RMZ

Element:
```

Notice here we have three nodal velocity components, a nodal pressure, and three more components of the residuals of the momentum equations.

4. Once we know what can be plotted lets first look at the mesh. This is default but can be forced at any time with the "wire" command:

DETOUR> wire DETOUR>p

These two commands will show you the mesh from a viewing angle parallel with the z-axis.

To rotate the view, use the rotate commands, viz.

```
DETOUR> rotate x 45
DETOUR> rotate y 45
DETOUR> p
```

5. Now let's look at the velocity vectors. To do this issue the commands:

DETOUR> vect vx vy vz DETOUR> p

You will notice the velocity vectors on the symmetry plane of the die, at Z=0.

There are ways to slice up the domain and look at so-called hedge-hog plots but those will not be covered here.

6. Now look at the contours of various variables over the surfaces:

```
DETOUR> contour pressure
DETOUR> p
DETOUR> vx
DETOUR> p
```

You will notice the contours in these series of the pressure and the x-component of velocity.

You can adjust the number of contours as follows:

```
DETOUR> ncntrs 40
DETOUR> p
```

And then you can paint the contours as follows:

```
DETOUR> paint
DETOUR> spectrum 40
DETOUR> p
```

Here you have specified 40 colors to the color spectrum.

```
Additional rotations can be performed; note that incremental rotations are all additive. Try DETOUR> rotate x -90
DETOUR> p
```

This rotates about the x-axis 90 degrees.

To reset all rotations and all other settings:

```
DETOUR> reset
DETOUR> p
```

To exit BLOT: DETOUR> exit

7. To obtain hard copies, you must generate a postscript file. First, recall that you saved a log file up above. This file was saved as 3ddie.blot.log. N.B. YOU MUST COPY THIS FILE INTO ANOTHER NAME BEFORE YOU START UP BLOT AGAIN, OR IT WILL GET BLOWN AWAY.

```
Issue the command
cp 3ddie.blot.log blot.log
```

Here you add a switch on the BLOT startup line: blot -device cps 3ddie.exoII Here we will re-execute all of the BLOT commands by loading the log file: BLOT> cmdfile blot.log

You will notice that BLOT automatically executes the commands in the log file, which we encourage you to look at, and exits automatically. List the files in the directory and you will notice a file called **3ddie.ps**. This is the postscript file that can be sent to a printer.

8. One final trick, and something that can be added to a Frequently Asked Questions (FAQ) list:

To remove all of the border axes, version information and frame of the plot in the postscript file so that the file might be cleanly imported into a wordprocessing document, can be accomplished in two ways. The first is to just do a screen capture of the plot while running BLOT in the X-window default mode. Most Unix systems have this capability, like **xwd** etc. which can produce a bit map file that can be cropped or edited. This approach is highly machine dependent. Some word processing software also supports this utility, like FrameMaker (capture command from the file utility menu).

Perhaps an easier way is to issue the following commands in DETOUR upon entering:

```
DETOUR> legend off
DETOUR> qa off
DETOUR> axis off
DETOUR> outline off
```

Any plotting performed subsequent to these commands will not have these features. You may want to leave the legend on and turn the others off.

9. Seriously, this is the last trick. When visualizing a transient data set, BLOT scales the min and max for contouring globally. This means if a field is evolving over time, e.g. a temperature is rising from zero to over 1000 deg. C, then the contours on all time planes are scaled from 0 to 1000. This means that on early time planes you will not see any variation if that variation is small relative to the {max T - min T}. To scale each time-plane on its own min and max, simply issue the following toggle:

DETOUR> cgl

I have no idea what "cgl" stands for.

## 6. Goma Introduction

This section is intended to give you a brief working introduction to Goma. In most cases, all information here can be found in the Goma user's manual and you are encouraged to have a close look at that and have it on hand as you go through this introductory tutorial. This section is more-or-less a synopsis of the manual. We will describe here the necessary details of each part of the input and material files. A separate chapter is devoted to each in the manual, so again this is intended to give you a quick feel for the input files. Reference to relevant sections of the manual are made in the clips from computer input files; these references will be seen as section numbers from the Goma manual in an italic font enclosed in parentheses near the right margin (e.g., *(section 4.1)*).

The first example on knife coating illustrates the use of APREPRO, multiple material conjugate problems, and a continuation strategy. The second problem is a substrate-film drying problem. This problem models a drying film on a flexible substrate which curls as a result of volume shrinkage. We run this in both a steady state and transient mode to demonstrate many additional features of Goma.

# 7. Goma TUTORIAL ON KNIFE COATING

In the tutorial directory there is a subdirectory called "knife". Change directories into knife and view the files. You will notice files called geometry and knife\_input. This first task is to discuss the details of these files, so you understand what it takes to run this problem. The file geometry actually serves two purposes: one is to define or parameterize the problem in terms of familiar quantities, like knife angle, bevel angle, coating speed, etc., and the second is to serve as a CUBIT (FASTQ) input file for the mesh. Recall from the APREPRO tutorial that you could make this two files: one "definitions" file and one CUBIT (FASTQ) input file. Using the APREPRO include statement, the definitions file could be incorporated (by reference) into the CUBIT (FASTQ) input, but in this case we have combined them. One could certainly convert this FASTQ input file to a CUBIT journal file. That exercise is left to the reader. The geometry file looks like this:

```
$Thermo-Physical Properties
                            (all units mks)
Ś
$ Base viscosity
                                   \{visc = 0.01\}
                             \{densi = 1.e3\}
$ density
                                 \{st = 0.03\}
$ surface tension
                             \{qrav = 9.8\}
$ gravity
Ś
Ś
$ GEOMETRY AND OPERATING CONDITIONS (MKS)
$ gap (leading edge to substrate) {Gap = 0.0005}
                                         \{d = 0.002\}
$ blade thickness
$ final thickness guess for geometry {Gap}
$ bevel angle of blade tip {alpha = PI/3.2} {alpha new = PI/3.2}
$ angle of blade face with gravity
                                         \{beta = PI/10\} \{beta new = PI/10\}
$ length of outflow plane
                                         \{S = 0.015\}
$ height of open boundary
                                        \{H = 0.006\}
$ distance from tip to inflow bndry
                                         \{I = 0.005\}
$ substrate thickness (for penetration) {h = 0.0004}
$ webspeed
                             \{websp = 0.1\}
$
$
  MESH PARAMETERS
$
${no elem along outflow = 7}
${no elem under blade = 7}
${no elem across layer = 4}
${no elem across inflow = 9}
${no elem across inflow back side = 6}
${no elem across pond = 6}
${no elem across substrate = 3}
${no elem along blade = 5}
        10 \{x10=-I\}
                          {y10=-h}
Point
```

```
Point
           11
                 \{x11=-0\}
                              {y11=-h}
Point
           12
                 \{x12=d*\cos(PI/2.-alpha-beta)\} {y12=-h}
Point
           13
                              {y13=-h}
                 {x13=S}
Point
           20
                 \{x20=-I\}
                              \{y20=0\}
           21
Point
                 \{x21=-0\}
                              {y21=0}
           22
                 \{x22=d*\cos(PI/2.-alpha-beta)\} {y22=0}
Point
           23
                              {y23=0}
Point
                 {x23=S}
Point
           30
                 \{x30=-I\}
                              {y30=Gap}
           31
Point
                 {x31=0}
                              {y31=Gap}
Point
           32
                 \{x32=d*\cos(PI/2. - alpha - beta)\} {y32 = d*sin(PI/2.-alpha-
beta) }
$$$$ {x32 new=d*cos(PI/2. - alpha new - beta new)} {y32 new = d*sin(PI/2.-
alpha new-beta new) }
Point
        33 {x33=s}
                        {y33=Gap}
Point
        40
                 \{x40 = -I\}
                              \{y40=H\}
        41 {x41=-(H-Gap)*tan(beta)} {y41=H}
Point
$ Kramers rule for the solution of two equations and two unknowns
$ is needed for the input of the line segments to salsa.
$
           10 STR
                         10
                               11
                                      0
                                           {no elem across inflow} 0.8
Line
Line
           11
                   STR
                         11
                               12
                                      0
                                           {no elem under blade} 1.
Line
           12
                  STR
                         12
                               13
                                      0
                                           {no elem along outflow} 1.2
Line
           20
                  STR 20
                               21
                                     0
                                           {no elem across inflow} 0.8
Line 21
           STR
                 21
                         22
                               0
                                     {no elem under blade} 1.
Line 22
           STR
                 22
                        23
                              0
                                     {no elem along outflow} 1.2
Line 40
           STR
                 40
                                     {no elem across inflow back side} 1.0
                        41
                              0
Line 31
                                     {no elem under blade} 1.
           STR
                 31
                        32
                              0
Line 32
           STR
                 32
                        33
                              0
                                     {no elem along outflow} 1.2
Line 100
           STR
                 10
                        20
                              0
                                     {no elem across substrate} 1.
Line 110
           STR
                 20
                        40
                              0
                                     {no elem across inflow back side} 1.
Line 120
           STR
                 41
                        31
                              0
                                     {no elem along blade} 0.8
Line
        200
                 STR
                         31
                                 21
                                          0
                                                   {no elem across layer} 1.
Line
        210
                 STR
                         32
                                 22
                                          0
                                                   {no elem across layer} 1
T.ine
        220
                 STR
                         33
                                 23
                                          0
                                                   {no elem across layer} 1
Line
        240
                 STR
                         23
                                 13
                                          0
                                                   {no elem across substrate} 1
$$REGION 4 2 -100 -10 -11 -12 -240 -22 -21 -20
REGION 1 1 -20 -200 -120 -40 -110
REGION 2 1 -200 -21 -210 -31
REGION 3 1 -210 -22 -220 -32
BODY 1 2 3
SCHEME 1 X
SCHEME 2 M
SCHEME 3 M
SCHEME 4 M
POINBC 100 32
POINBC 200 33
NODEBC {substrate ns=2} 20 21 22
```

```
NODEBC {inflow_back_ns=3} 110
NODEBC {inflow_top_ns=4} 40
NODEBC {blade_face_ns=5} 120
NODEBC {blade_tip_ns=6} 31
NODEBC {outflow_plane_ns=8} 220
ELEMBC {substrate_ss=2} 20 21 22
ELEMBC {inflow_back_ss=3} 110
ELEMBC {inflow_top_ss=4} 40
ELEMBC {blade_face_ss=5} 120
ELEMBC {blade_tip_ss=6} 31
ELEMBC {free_surface_ss=7} 32
ELEMBC {outflow_plane_ss=8} 220
```

#### EXIT

Notice how the points and the lines are expressed in terms of the defined parameters like blade thickness, gap, bevel angle, etc. Also notice that we have defined names for each ELEMBC, or side set, and each NODEBC, or node set. That is, after this file is processed with APREPRO those names are just converted into numbers, but including this file in the Goma input file allows us to refer to the side set and node set numbers by name.

1. Let us go ahead and process this file into a mesh. To do this, we need to read it into FASTQ, but not before we process it through APREPRO, viz.

```
cubit
CUBIT> import fastq 'geometry'
CUBIT> mesh surface all
CUBIT> block 1 surface all
CUBIT> block 1 element type QUAD9
CUBIT> export genesis 'knife.exoII' overwrite
(one could do the same with fastq, following the instructions in APPENDIX
A):
fastq -a geometry
ENTER OPTION: m,ni,op,p,g,p
ENTER MESH GRAPHICS OPTION: ,w
GENESIS DATABASE OUTPUT FILE NAME: knife.gen
ENTER MESH OPTION: exit
```

(Note here that we turned on the nine-node quad option with **ni**, and the optimize option with **op**. These options are toggle switches, and can be put into the FASTQ input file as a **NINE** and a **RENUM** card, respectively. Make sure you have generated a nine-node quad mesh, i.e, make sure FASTQ tells you this:

**	MESH PROCESSING COMPLETED	**
**	THREE NODE BARS OUTPUT	**
**	NINE NODE QUADS OUTPUT	**
**	WITH NODE AND ELEMENT NUMBERING OPTIMIZED	**
**	LARGEST NODE DIFFERENCE PER ELEMENT: 52	**
**	NODES: 427; ELEMENTS: 92; MATERIALS: 1	**
**	***************************************	***

In CUBIT (FASTQ), have a look at the geometry by executing it. Notice that we have a knife, a pond upstream of the knife, and a well-defined substrate. As it turns out, the substrate is Region 4, and we currently have that region commented-out in the file (see the first <u>double underlined</u> region card above). That is, we are not going to solve any equations in the substrate. As an extension to this exercise, though we will grid up the substrate and allow it to deform for now. The annotated initial meshed geometry is show below.



 Now we will dissect the Goma input file to make sure we are defining correctly the problem to be solved. In the tutorial/knife subdirectory, you will notice the file knife\_input. Either "more" or "vi" this file and examine it.

The first section looks like this

{include(geometry)}

FEM File Specif	ications	(Section 4.1)
FEM file	<pre>= knife.exoII</pre>	
Output EXODUS II file	= out.exoII	
GUESS file	= contin.dat	
SOLN file	= soln.dat	
Write intermediate results	= no	
General Specifi	cations	
Number of processors	= 1	(Section 4.2)
Output Level	= 0	
Debug	= 0	
Initial Guess	= zero	

Notice that the "geometry" file discussed above is included here, so that several important parameters regarding geometry and properties can be calculated. The highlights of this section of the Goma input deck are that we are taking the mesh from the file knife.exoII, writing the results to out.exoII, and using a zero initial guess. The next two sections are as follows:



Since we have chosen "steady" for time integration, The "Time Integration Specification" section is completely specified. For transient simulation, we need to specify more entries such as time integration scheme, initial time step, final time, etc. The solution algorithm for the matrix system that results from the Newton iteration scheme is "umf" which comes from direct solver UMFPACK. Other options for direct solvers are "lu", and "amesos". Amesos is an interface Goma used to access parallel direct solvers such as SuperLU and MUMPS. See Goma's user manual for more details. Iterative solvers are available as well; however, their use for viscous free surface flows requires pressure stabilization options beyond the scope of this discussion. The preconditioner cards, polynomial cards, size of Krylov subspace and Orthogonalization cards and Linear solve iteration cards are all ignored with the "umf" option. The "Number of Newton Iterations" card sets the maximum number of nonlinear iterations. The Newton correction factor for each Newton iteration. Conveniently, these can be overridden from the Goma execute command line, as described in the manual and demonstrated below. This is handy when making several continuation steps to get within the radius of convergence.

The next relevant section is the all-important boundary condition section:

```
Boundary Condition Specifications
Related SS bc's on position
$ SET c's to zero for 2D problem
$ {c1=0} {c2=0} {c3=0} {c4=0} {c5=0} {c6=0} {c7=0} {c8=0}
$
$ Calculate coefficients for general equation a*x + b*y +c*z +d = 0
$ { {a2=(y20-y23)/(x23-x20)} { { { { { { { { { { { { } { { { } { { { } { { { } { { { } { } { { { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } { } } } } } } } } } } } } } } } } } }
```

```
$ {b2=1}
$
$ NB: this is a vertical line
  \{b3=(x20-x40)/(y40-y20)\}
$
$
   {d3=-x40-b3*y40}
   {a3=1}
$
$ NB: this could be a vertical line
   \{b5=(x41-x31)/(y31-y41)\}
$
$
  {d5=-x31-b5*y31}
$
   {a5=1}
$
$
  {a6=(y31-y32 new)/(x32 new-x31)}
$
   {d6=(-y32 new-a6*x32 new)}
```

\$ {b6=1}

Number of BC = -1 = PLANE SS 2  $\{a2\}$   $\{b2\}$   $\{c2\}$   $\{d2\}$ BC BC = PLANE SS 3 {a3} {b3} {c3} {d3} BC = PLANE SS 4 0. 1. 0.  $-\{H\}$ BC = PLANE SS 5 {a5} {b5} {c5} {d5} BC = PLANE SS 6 {a6} {b6} {c6} {d6} BC = PLANE SS 8 1. 0. 0.  $\{-S\}$ BC = U NS 2 {websp} BC = V NS 2 0. BC = V NS 3 0. BC = V NS 4 0. BC = U NS 5 0. = V NS 5 0.BC BC = U NS 6 0. BC = V NS 6 0.BC = VELO NORMAL SS 7 0. = KINEMATIC SS 7 0. \$\$BC = CAPILLARY SS 7 1. 0. 0. 0. \$\$BC \$\$BC = CAP\_ENDFORCE NS 200 1. 0. 0. 1.0 \$BC = V NS 8 0.BC = VELO TANGENT SS 8 0 0. 0. 0.  $BC = DX NS 100 \{x32 new - x32\} 1.0$ BC = DY NS 100 {y32\_new - y32} 1.0

END OF BC

Here we will discuss the <u>double-underlined</u> cards in this section, as they are the most important.

• The first set of cards is used to compute the slopes and intercepts of the straight lines used to define

the geometry. These coefficients are needed on the PLANE geometric boundary conditions below. Notice how these coefficients depend on the geometrical point locations that were defined with APREPRO in the geometry file.

- The next line with a double underline is the <u>Number of BC</u> = -1 card. Here you can either specify the number of boundary condition cards to be read, or just specify -1, in which case it will read all BC cards between it and the END OF BC card.
- The first set of BCs pertains to the geometry. The PLANE boundary conditions specify that the mesh along that plane must remain on the plane, but may slide frictionlessly along it. Note that the coefficients depend on the original geometry, but that the geometry may be changed without regenerating the mesh, as shown below.
- Note that the <u>BC = U NS 2 {websp}</u> card specifies that the x-component of velocity along the substrate is set at the web speed, defined in the geometry file. This substrate is node set 2. To verify quickly that this is node set 2, run BLOT as follows:

```
blot knife.exoII
det
nset 2
p
```

• The next set of highlighted cards contains the VELO\_NORMAL condition and the KINEMATIC condition. The first step of obtaining a solution here is to do so on a fixed grid. In this case we need to comment out the KINEMATIC card (note that we use \$\$ in the first two columns, but you can do whatever you want), and solve the equations with the VELO\_NORMAL boundary condition. The VELO\_NORMAL condition specifies that no penetration is allowed across that side set (in this case side set 7) but in the absence of any other conditions allows the fluid to slip freely along the side set. Run BLOT again to verify that this is the downstream meniscus:

```
blot knife.exoII
det
sset 7
p
```

- Below we will change out the VELO\_NORMAL condition for the KINEMATIC condition when we allow the surface to go free.
- Finally the CAPILLARY card and the CAP\_ENDFORCE card are used to apply surface tension to the surface. We will demonstrate these below.

```
•
```

The next relevant section is that of the Problem Description:

```
###########
Problem Description
                                                       (Section 4.12)
_ _ _
Number of Materials = 1
MAT = coating liq
                   1
   Coordinate System = CARTESIAN
   Mesh Motion = ARBITRARY
   Number of bulk species = 0
                            = 5
   Number of EQ
                  Q1 D1
   EQ = mesh1
                                      0.
                                          0.
                                              0.
                                                   1.
                                                         Ο.
                           Q1
   EQ = mesh2
                  Q1 D2
                           Q1
                                      0.
                                          0.
                                              0.
                                                   1.
                                                         0.
   EQ = momentum1 Q2 U1
                           Q2
                                      0. 1.
                                              1.
                                                   1.
                                                         0. 0.
   EQ = momentum2 Q2 U2
                                      0. 1.
                           Q2
                                              1.
                                                   1.
                                                         0. 0.
   EQ = continuity P1 P
                           Р1
                                                         0.
                                 1.
                                 div ms
                                        adv bnd dif src porous
```

- 25 -

Notice here that the material file from which Goma will seek the material properties is called **coating\_liq.mat**. Also notice that the block number is 1, and this number corresponds to the material number input on the **region** card in FASTQ. By the way, you should have a look at this material file to see how the properties are input. Also notice that this is a **CARTESIAN** simulation with **ARBITRARY** mesh motion. Rather than go into details here, please refer to the manual for the purpose of these cards. What is important to point out here, however, is the number of equations and materials. In this simulation, we have one material (**coating\_liq.mat**) in which we will solve 5 differential equations. The two mesh equations (**mesh1** and **mesh2**) are needed to move the mesh as a pseudo-solid. Notice that we use one-order lower basis functions for the mapping, while maintaining a biquadratic element for the velocities, i.e., **Q2**. The names of the variables **U1**, **U2**, **D1**, **D2**, and **P** are not arbitrary, so please adhere to what the manual allows for now.

Finally, the floating point constants on the equation specification lines are term multipliers, which are mainly used for research purposes. These multipliers are typically set to zero or one, depending on whether you want the term on or off. Each column of multipliers refers to a particular term, as indicated by the "div ms adv bnd..." comment line. Actually, if any physical property multiplies a term, like density on a convective term, the multiplier also multiplies the same term. i.e., it is not recommended to use these terms to input physical properties, although one could.

The remainder of the Goma input deck specifies output for the resulting EXODUS II file, out.exoII in this case, including specific user-selected auxiliary fields that will be computed. You can read about these cards in the manual.

3. Now it is time to run this knife coating problem. First we will get a solution on a fixed grid. For this we will leave the knife\_input file as is and execute:

Goma -a -i knife\_input

Note that we use the -a switch to head knife\_input and coating\_liq.mat through APREPRO before Goma. After several screens worth of informational junk which we will eventually put into a file, you will see:

```
Number of unknowns
                        = 1374
Number of matrix nonzeroes = 70646
                               Correction
            Residual
       itn Loo L1 L2
                               Loo L1 L2 lis asm/slv (sec)
 TOD
17:13:35 [0] 2.2e-04 7.6e-03 7.8e-04 2.5e+01 9.2e+02 1.2e+02 1 2.2e-01/5.0e-02
17:14:05 [1] 1.6e-04 5.8e-03 5.4e-04 2.0e+00 7.2e+01 7.7e+00 1 1.8e-01/4.0e-02
17:14:14 [2] 3.6e-05 1.3e-03 1.4e-04 6.3e-02 2.9e+00 2.8e-01 1 1.8e-01/3.0e-02
17:14:23 [3] 6.7e-07 1.9e-05 2.2e-06 1.3e-03 7.1e-02 7.1e-03 1 1.9e-01/3.0e-02
17:14:32 [4] 2.1e-10 5.5e-09 6.4e-10 6.8e-07 4.0e-05 4.1e-06 1 1.9e-01/3.0e-02
17:14:40 [5] 1.5e-17 5.3e-16 5.2e-17 3.5e-14 2.2e-12 2.1e-13 1 1.9e-01/3.0e-02
-done
```

Note the strong convergence in all norms, both the Residual norms (the first 3 columns) and the Newton update norms (columns 4 through 6). The numbers under the asm/slv (sec) column are the cpu time it takes to assemble the residual equations and solve the resulting matrix system, respectively. You should look at this result quickly with:

```
blot out.exoII
det
vect vx vy
p
cont stream
p
```

4. The next step is to do a little zeroth order continuation to release the meniscus and get a free surface flow. Notice that the continuation file in the knife\_input deck is soln.dat. To read it in, copy soln.dat into contin.dat and edit the input file Initial Guess card to reflect "read", i.e.,

```
Initial Guess = read
```

We also need to release the free surface. To do this comment out the **VELO\_NORMAL** card and uncomment the **KINEMATIC** card in the **Knife\_input** file, i.e., change this

```
BC = VELO_NORMAL SS 7 0.

$$BC = KINEMATIC SS 7 0.

$$BC = CAP_ENDFORCE NS 200 1. 0. 0. {st}

to

$$BC = VELO_NORMAL SS 7 0.

BC = KINEMATIC SS 7 0.

BC = CAP_ENDFORCE NS 200 1. 0. 0. {st}
```

Save the file.

Goma -a -i knife\_input -r 0.1 -n 7

followed by five steps of -r 0.8 Newton iteration (notice the use of the -n option to override the specification of the Max. Number of Newton Iterations in the input deck):

```
cp soln.dat contin.dat
Goma -a -i knife_input -r 0.8 -n 5
```

followed by a few steps of full Newton:

cp soln.dat contin.dat Goma -a -i knife\_input

Now look at the results and you will see that the surface has "sagged" and you now have a development zone.

```
blot out.exoII
det
cont stream
p
```

5. Now we will alter the geometry a bit, without regenerating the original mesh. First, change the bevel angle of the blade in the geometry file:

Change

```
$ bevel angle of blade tip {alpha = PI/3.2} {alpha_new = PI/3.2}
to
  $ bevel angle of blade tip {alpha = PI/3.2} {alpha_new = PI/4.2}
Let us first try a full Newton step:
   cp soln.dat contin.dat
   Goma -a -i knife_input
```

Notice again the strong convergence. Have a look at the results again with BLOT and notice that the bevel face is much steeper.

# **Goma TUTORIAL ON FILM DRYING-SUBSTRATE CURL**

For this problem you need to change directories into \$ (TUTORIAL) /tutorial/curl, where \$(TUTORIAL) is an environment variable defined for the header directory. Listing (ls) files in that directory shows the following:

coating.mat	out_steady.exoII	<pre>tmp.coating.mat</pre>	trans_output
film.exoII	out_trans.exoII	tmp.input	
input_steady	soln.dat	<pre>tmp.substrate.mat</pre>	
input_trans	substrate.mat	trans_error	

Here there are two Goma input files: input\_steady and input\_trans. We will discuss each case. Also notice the tmp.\* files. These files are produced when using the -a switch on the Goma run command. You can always delete these files to clean up the directory. We will first generate a mesh, or CUBIT/FASTQ file for the problem (film.exoII) using the approach you have learned in previous examples. The CUBIT/FASTQ input file corresponds to the following geometry:



and has an input file (film.fas) that looks like:

TITLE							
SUBSTRATE	CURI	PROBLE	м				
POINT	1	0.00	00000E	+00	0.0	0000	000E+00
POINT	2	1.00	0000E	+01	0.0	0000	000E+00
POINT	3	1.00	00000E	+01	1.0	0000	000E+00
POINT	4	0.00	00000E	+00	1.0	0000	000E+00
POINT	5	0.00	00000E	+00	-5.0	0000	000E-01
POINT	6	1.00	00000E	+01	-5.0	0000	000E-01
LINE	1	STR	1	2	0	10	0.7000
LINE	2	STR	2	3	0	8	1.0000
LINE	3	STR	3	4	0	10	1.4200
LINE	4	STR	4	1	0	8	1.0000
LINE	5	STR	1	5	0	2	1.0000
LINE	6	STR	5	6	0	10	0.7000
LINE	7	STR	6	2	0	2	1.0000
REGION	1	1	-1	-2	-3	-4	
REGION	2	2	-6	-7	-1	-5	
SCHEME	0 м						

BODY	1	2
POINBC	100	1
POINBC	200	2
POINBC	300	3
POINBC	400	4
POINBC	500	6
POINBC	600	5
NODEBC	1	1
NODEBC	2	2
NODEBC	3	3
NODEBC	4	4
NODEBC	5	7
NODEBC	6	6
NODEBC	7	5
ELEMBC	1	1
ELEMBC	2	2
ELEMBC	3	3
ELEMBC	4	4
ELEMBC	5	7
ELEMBC	6	6
ELEMBC	7	5
RENUM		
NINE		
EXIT		

Notice there are two regions and two materials (see **REGION** cards) and the stretching coefficients that are used to draw the mesh to the outer edge of the film. The problem here is to clamp the inner edge of the coating and substrate (left side), dry the film, and follow the overall stress development and deformation. We will run this problem in two modes. First is the steady state mode. The input deck for this mode is the file input\_steady. Let's discuss some of the critical parts of that input file. In the first two sections, two cards are noteworthy:

FEM File Specifications		(Section 4.1)
FEM file	= film.exoII	
Output EXODUS II file	<pre>= out_steady.exoII</pre>	
GUESS file	= contin.dat	
SOLN file	= soln.dat	
Write intermediate results	= no	
General Specifications		(Section 4.2)
Number of processors	= 1	
Output Level	= 0	
Debug	= 0	
Initial Guess	= zero	
#Initial Guess	= read_exoII	
#Initial Guess	= read	
Initialize = MASS_FRACTION 0 0.2	5	

The input finite element database file (film.exoII) is defined on the FEM File card and the initial mass fraction of component 0 is set to 0.25 with the Initialize card. The next relevant section of input is boundary condition specification. (Since the problem is being run in the steady state mode with the umf solver, all other sections are like those in the previous case study. The boundary conditions look like:

```
____
Boundary Condition Specifications
                                                     (Section 4.10)
____
Number of BC
                               -1
                           =
BC = PLANE SS 4 1.00 0.0 0. 0.0
BC = DX NS 100 0.0
BC = DY NS 100 0.0
BC = PLANE SS 7 1.00 0.0 0.
                           0.0
BC =
       YFLUX SS 3 0
                                      0.25
                               5.
                     2
                           0 5.
BC =
       YFLUX
              SS
                                      0.25
#########
END OF BC
#########
```

Note here that we are pinning node set (i.e. NS) 100 with the DX and DY conditions. This is point 1 in the geometry file and is identified in film.fas as the first POINBC card. You can confirm this by looking at film.exoII with BLOT and turning on display of nset 100. Also, we are constraining side sets 4 and 7 (SS 4 and 7; see file film.fas) to stay on the x=0 plane with the PLANE boundary condition; this is the "clamped" end. Finally, we are specifying a lumped parameter mass-transfer model along the surface of the film so that the mass flux of Species 0 follows a 5.0\*(Concn - 0.25) specification at the surface.

The next section, or problem description section, contains several instructive features:

```
Problem Description
                                                      (Section 4.12)
Number of Materials = 2
MAT = coating
                  1
 Coordinate System = CARTESIAN
 Element Mapping
                = isoparametric
 Mesh Motion = LAGRANGIAN
 Number of bulk species = 1
   Number of EQ = 4
    EQ = mesh1
EQ = mesh2
                    Q2 D1 Q2
                                              Ο.
                                 0. 0.
                                                   1.
                                                       Ο.
                                                   1.
                    Q2 D2 Q2
                                    0. 0. 0.
                                                       Ο.
    EQ = continuity P1 P P1 1.
                                                       1.
    EQ = species bulk Q2 Y Q2
                              1. 1.
                                        1. 1. 0.
                               div
                                     ms adv bnd dif src porous
MAT =
        substrate
                    2
 Coordinate System = CARTESIAN
 Element Mapping = isoparametric
 Mesh Motion = LAGRANGIAN
 Number of bulk species = 0
   Number of EO = 3
    EQ = mesh1Q2D1Q2EQ = mesh2Q2D2Q2
                                   0. 0. 0.
                                                   1.
                                                       Ο.
                                    0. 0. 0.
                                                  1.
                                                       Ο.
    EQ = continuity P1 P P1
                              1.
                                                        1.
                               div ms adv bnd dif src porous
```

You'll notice that the evolution equations for the coating do not include solution of the momentum equations for the fluid. This is a solid film/coating which can support a shear stress. There are two materials, each with a different problem description - a truly conjugate problem. Note that Species 0 is confined to the film only and even though we might have more than one species, we use only one species\_bulk equation. The material files will single out properties of individual species, as discussed below. The continuity equation contains a source term; this is included in the formulation to account for the volume shrinkage effect produced by mass loss and to properly account for the pressure. The mesh motion type is Lagrangian, meaning the mesh moves with the materials. When the mesh motion is Lagrangian, it will deform according to the prescribed loads and according to the prescribed constitutive equation in the material file.

There are two materials, and so there MUST be two material files: substrate.mat and coating.mat. Let us examine each one (use more coating.mat and more substrate.mat). First, in coating.mat, you will notice the solid constitutive equation and the properties:

Mechanical Properties and Con	nstitutive Equati	ons (	Section 5.2)
Solid Constitutive Equation	= INCOMP_PSTRAIN		
#Solid Constitutive Equation	= HOOKEAN_PSTRAI	N	
Convective Lagrangian Velocity	= NONE		
Lame MU	= CONSTANT	1.	
Lame LAMBDA	= CONSTANT	0.	
Stress Free Solvent Vol Frac	= CONSTANT	0.5	

The constitutive equation is **INCOMP\_PSTRAIN**, i.e., incompressible plane strain. The fact that it is incompressible necessitates the solution of the continuity equation and the pressure unknowns. The **Lame MU** and **Lame LAMDA** coefficients are actually Poisson's ratio and the bulk modulus when using nonlinear constitutive equations. You'll notice the shear modulus is zero because the constitutive equation is incompressible. **Lame MU** then becomes Young's modulus.

Finally, the stress-free solvent volume fraction is set to 0.5; this is simply the solvent volume fraction at which the film is stress free.

The only other significant input in the coating.mat file to discuss is that which specifies the species diffusivity:

Species Properties					(Section 5.6)
Diffusion Constitutive Equation	=	FICKIAN			
Diffusivity	=	CONSTANT	0	1.	
Latent Heat Vaporization	=	CONSTANT	0	Ο.	
Latent Heat Fusion	=	CONSTANT	0	0.	
Vapor Pressure	=	CONSTANT	0	0.	
Species Volume Expansion	=	CONSTANT	0	1.	
Reference Concentration	=	CONSTANT	0	0.	

Note that the species number is 0 and the value is 1. If you had more than one species, you would repeat this group of cards.

In the substrate.mat file, you will notice that the same constitutive equations are employed and that the substrate is treated as incompressible but with a much higher modulus:

Solid Constitutive Equation	= INCOMP_PSTRAIN
Convective Lagrangian Velocity	= NONE
Lame MU	= CONSTANT 100.
Lame LAMBDA	= CONSTANT 0.
Stress Free Solvent Vol Frac	= CONSTANT 0.

Now let us run the steady and transient problems as identified in the 5 steps below:

1. First generate the mesh:

```
CUBIT> import fastq `film.fas'
CUBIT> mesh surface all
```

CUBIT> block 1 surface 1 CUBIT> block 2 surface 2 CUBIT> block 1 2 element type QUAD9 CUBIT> export genesis `film.exoII'

```
OR WITH FASTQ:
fastq -a film.fas
ENTER OPTION: m,p,g,p
ENTER MESH GRAPICS OPTION: ,
ENTER MESH OPTION: w
GENESIS DATABASE OUTPUT FILE NAME: film.gen
ENTER MESH OPTION: exit
```

2. Run Goma:

Goma -i input\_steady

3. Look at results:

```
blot out_steady.exoII
det
p
```

```
cont y0
```

(you will notice that there is no variation in concentration since we are at steady state conditions) cont e22

```
p
cont t11
p
exit
```

This is a steady version of the curl problem. The stresses in the film are sustained by resistance of the substrate to deformation. We can run this problem in a transient fashion and watch the concentration profiles develop. To do this, you must use the Goma input deck called input trans in the same directory. Issue the following UNIX diff command:

```
diff input_steady input_trans
```

```
and you will see
   5c5
   < Output EXODUS II file = out_steady.exoII
   _ _ _
   > Output EXODUS II file
                                    = out trans.exoII
   18c18
   < Initialize = MASS_FRACTION 0 0.25
   > Initialize = MASS FRACTION 0 0.5
   22c22,30
   < Time integration
                                     = steady
   _ _ _
   > Time integration
                                    = transient
                                     = 1.0e-3
   > delta_t
```

> Maximum	n number	of tim	e steps	= 3	100						
> Maximum	= 10.0e+0										
> Minimum	n time s	tep		= 3	1.0000	e-9					
> Time step parameter					0.0						
> Time st	ep erro	r		= (	0.002	1	1	1	1	1	1
> Printir	ng Freque	ency		= 3	1						
44,45c52,	53										
< BC =	YFLUX	SS	3	0	5.	Ο.	25				
< BC =	YFLUX	SS	2	0	5.	Ο.	25				
> BC =	YFLUX	SS	3	0	5.	Ο.					
N BC -	VELUX	66	2	0	Б	Δ					

The differences are clear. We are specifying a higher stress-free solvent volume fraction (MASS\_FRACTION) and a lower "sink" concentration on the mass transfer coefficient (YFLUX). Also notice that the Time Integration card was switched to transient and we then supply all the relevant time integration information. You should consult your manual for the purpose of each card.

4. To run the transient version:

Goma -i input\_trans

You will notice standard output (to your screen) which looks like:

```
Number of unknowns
                           = 1539
Number of matrix nonzeroes
                           = 81641
   Setting MASS FRACTION number 0 (variable [4]) to 0.5
=> Try for soln at t=0.001 with dt=0.001 [0 for 0] (BE)
   Newton Convergence - Implicit
                                                      Time
                                                               Step
                   L 1
 ToD
        itn Loo
                           L_2
                                   L 00
                                          L_1
                                                 L_2 lis asm/slv (sec)
        --- ----- ----
                                                 _____ ___ ___
16:32:56 [0] 2.1e-02 9.1e-01 1.1e-01 1.0e+00 8.5e+01 8.9e+00 1 2.4e-01/1.6e+00
16:32:58 [1] 2.0e-03 4.2e-02 5.2e-03 2.3e-01 1.8e+01 8.1e-01 1 2.1e-01/3.4e-01
16:32:59 [2] 5.9e-04 6.3e-03 1.1e-03 2.3e-02 5.6e-01 4.1e-02 1 2.2e-01/2.0e-01
16:32:59 [3] 3.6e-05 2.0e-04 6.0e-05 1.5e-03 2.4e-02 2.1e-03 1 2.1e-01/1.9e-01
16:32:59 [4] 1.8e-07 7.0e-07 2.6e-07 1.2e-05 3.8e-05 1.4e-05 1 2.2e-01/1.9e-01
16:33:00 [5] 4.3e-12 1.8e-11 6.0e-12 2.6e-10 8.3e-10 3.4e-10 1 2.2e-01/1.9e-01
16:33:00 [6] 4.0e-16 1.2e-14 1.0e-15 3.4e-14 1.0e-12 1.1e-13 1 2.1e-01/2.0e-01
scaled solution norms 1.013227e+00 1.777290e-01 3.300731e-01
CONSTANT DELTA T
                       [1.1e-02, 4.1e-03, 1.3e-01]
Predictor-corrector norm: [ 1 d , 1 y ,
                                          1 P 1
=> Try for soln at t=0.002 with dt=0.001 [1 for 1] (BE)
   Newton Convergence - Implicit
                                                      Time Step
     itn Loo Ll
                          ь 2
                                   Loo L1
                                                L 2 lis asm/slv (sec)
 ToD
   _____ ___ _____ _____ _____ _____ _____
16:33:01 [0] 1.3e-02 7.1e-01 7.4e-02 1.0e+00 8.1e+01 8.9e+00 1 2.1e-01/1.9e-01
```

16:33:01 [1] 2.0e-04 5.4e-03 6.7e-04 9.8e-03 3.3e+00 1.5e-01 1 2.1e-01/1.9e-01 16:33:02 [2] 1.8e-06 2.9e-05 3.6e-06 7.6e-05 1.3e-02 5.5e-04 1 2.1e-01/2.0e-01 16:33:02 [3] 4.0e-10 2.0e-09 5.7e-10 1.9e-08 4.5e-06 2.1e-07 1 2.1e-01/2.0e-01 16:33:02 [4] 3.5e-16 1.3e-14 9.5e-16 5.9e-14 1.8e-12 1.4e-13 1 2.1e-01/2.0e-01 scaled solution norms 1.026663e+00 1.858727e-01 3.301558e-01 CONSTANT DELTA T [2.2e-03, 2.4e-03, 1.3e-01] Predictor-corrector norm: [ 1 d , 1 y , 1 P ]  $\Rightarrow$  Try for soln at t=0.003 with dt=0.001 [2 for 2] (BE) Newton Convergence - Implicit Time Step ToD itn Loo L1 L2 Loo L1 L2 lis asm/slv (sec) ----- --- ----- ------16:33:03 [0] 1.8e-03 9.0e-02 1.0e-02 1.3e-02 1.4e+00 6.5e-02 1 2.1e-01/2.0e-01 16:33:03 [1] 1.8e-05 3.8e-04 4.0e-05 1.9e-04 1.4e-02 6.1e-04 1 2.1e-01/2.0e-01 16:33:04 [2] 4.1e-09 1.4e-08 4.8e-09 4.0e-08 4.8e-07 4.6e-08 1 2.1e-01/2.0e-01 16:33:04 [3] 5.2e-16 1.5e-14 1.2e-15 5.8e-14 1.4e-12 1.8e-13 1 2.1e-01/2.0e-01 scaled solution norms 1.039568e+00 1.934510e-01 3.310054e-01

The time step starts as 1.e-3 but adjusts (grows or is reduced) according to the error measure defined by the **Time Step Error** card. When you look at the results with **blot**, which are in file **out\_trans.exoII**, notice that contouring the concentration (**vo**) shows the development of concentration boundary layers, as expected. Also notice that all of the time planes are output into the EXODUS II file. You can control this with the printing frequency card.

There is much more to glean from all exercises in this tutorial and this document will be continually updated (see version number on Subject line). This serves as an introduction to Goma and its associated pre- and post-processors. Questions may be addressed to Randy at prschun@sandia.gov.

## **APPENDIX: FASTO, GJOIN, GEN3D**

This section introduces and provides a tutorial on mesh generation with FASTQ, GEN3D and GJOIN, and subsequent database manipulation/interrogation with GROPE and ALGEBRA. You can read about each of these tools in your SEACAS documentation, as a Sandia Technical Report for each is contained in that set.

FASTQ is a straight forward two-dimensional mesh generator. It has the ability to produce meshes on arbitrary shaped domains with both mapped and paved meshes. FASTQ is needed to generate the input mesh file (an EXODUS II file) for Goma. The tutorial below will instruct you how to do this. As a take-home assignment here, locate the FASTQ FLOWCHART figure on page 21 of the FASTQ user's manual illustrating the layered command structure. Make a photocopy of that page and paste it on your wall next to your computer. This page is easily the most valuable reference in the manual. NOTE: Since about 2002 FASTQ is rarely used as a mesh generator as several mainstream geometry-CAD based mesh generators like PATRAN<sup>TM</sup>, Solid Works<sup>TM</sup>, and Sandia's product and now commercially available CUBIT. Nonetheless, it is useful to be aware of FASTQ's capabilities in case you are ever on a computer without access to these high-end mesh generators.

Regarding the cheat sheet, you will notice on the page that the command structure is "layered". When you start FASTQ, you are in the top (left most) layer. There you can do a number of things. To see what these are just look at the cheat sheet, or type "help". At all layers, you can type "help" or "?" to get the list of commands expected. Typing a command (typically just its first letter or first two letters) which selcts an option (versus one that executes a function), sends you down into that layer. To go up a layer, just hit return or place an extra comma at the beginning of a string of commands. The tutorial below illustrates this.

Once you have written an EXODUS file (actually, it is a Genesis file and as of 4 March 1997, it is in an EXODUS I format. This means you have to run **ex1ex2v2** to convert it to **exoII** format for reading by Goma.), you can use GEN3D to extrude, rotate, warp, etc. the mesh into a 3D mesh. You can also join multiple 3D meshes with GJOIN to make still more complicated meshes. The tutorial below will show you how to do this.

*IMPORTANT NOTE:* You are not restricted to using FASTQ/GEN3D/GJOIN to generate meshes for Goma. You can use PATRAN and CUBIT. Please contact Randy Schunk (prschun@sandia.gov, 505-844-5992) for more details.

### FASTO/GEN3D/GJOIN TUTORIAL

There are several ways in which to run FASTQ. One is in interactive mode with all input from the command line; a second is in interactive mode, with the commands being taken from an input file; a third way is in batch mode with the commands also coming from an input file.

Again you should be in the tutorial subdirectory to demonstrate this. Let's first mesh up a 2D box (i.e. square):

1. Issue the command:

fastq

You will notice a window pop up. Now issue the command "help" and you will see the options available to you on this level.

 The first step is to input the solid geometry. To do this enter the "keyin" layer: keyin (or just "k" and enter)

Again type "help" and notice all of the entities available. To define a geometry, we need points, lines, and regions. Start with points:

p\*oint (i.e., you can just say "p")

You will notice the following:

ENTER KEYIN OPTION: p ENTER POINT DATA IN THE FOLLOWING FORMAT: [ POINT NO., X, Y ] HIT RETURN TO END INPUT Begin entering your points as follows (corners of a unit square):

Here we have points 1 through 4 with coordinates (0,0), (1,0), (1,1), and (0,1) respectively. To see these points graphically:

,g,p

Note here the first comma takes you up to the top level, the g takes you into the graphics level, and the p plots the points. Note that you could have just as easily entered a "return" instead of a comma and then a g, p. Alternatively, you can enter each command separated by a return.

Now go back to the keyin mode with

, k

Now we will enter the connecting lines:

```
l*ine (you enter this and FASTQ responds with the following)
THE FOLLOWING LINE TYPES ARE AVAILABLE:
    S*TRAIGHT = STRAIGHT LINE
    CI*RCULAR = CIRCULAR CCW ARC ABOUT A CENTER
    3*CIRCULAR = CIRCULAR ARC WITH 3RD ARC POINT
    R*CIRCULAR = CIRCULAR ARC WITH RADIUS
    E*LIPSE = CCW ELIPSE ABOUT A CENTER
    CO*RNER = 2 LINE SEGMENTS JOINED
    P*ARABOLA = PARABOLIC SHAPED LINE
WHICH LINE TYPE WOULD YOU LIKE TO ENTER:
```

Obviously we want straight lines for a box so enter "s" and you will get

ENTER STRAIGHT LINE DATA IN THE FOLLOWING FORMAT: [ LINE NO., POINT 1, POINT 2, NO. INTERVALS, FACTOR ] HIT RETURN TO END INPUT >

Now enter the four connecting lines with 2 intervals on each line (FACTOR defaults to 1).

To see this geometry, again enter

,g,p

Now go back to the keyin mode to enter the region, side set and node set info:

,k,r
ARE YOU USING SIDES IN DEFINING REGIONS?

Type "no" for this case, because sides are defined as a collection of lines. In this case we will define our region with a collection of lines.

```
ARE YOU USING SIDES IN DEFINING REGIONS? no
ENTER REGION DATA IN THE FOLLOWING FORMAT:
[ REGION NO., MATERIAL NO., LINE 1, LINE 2, ..., LINE N ]
HIT RETURN TO END INPUT
>
```

In response to this just list out the region number, the material number, and the lines in a continuously connected circuit:

>1 1 1 2 3 4

Note here that the region label is "1" and the material label is also "1". These are just names or labels used in the Goma input deck to reference regions, each of which may have a different number of defining equations, etc.

3. We are now ready to generate a mesh. "Return" up a level and using the "help" command, locate the "M\*ESH" command for generating the mesh. Alternatively enter:

Now enter "s" to begin (step) processing and follow the prompts. You should read about all of the options for meshing standard primitives etc. within the FASTQ manual. For this tutorial, enter the following sequence where your response to the prompt is indicated by a double underline (\_): ENTER OPTION: m, s

```
MESH PROCESSING BEGUN
                                  1
 INITIAL CHECK BEGUN FOR REGION:
 STEP PROCESS REGIONS I1 THROUGH I2
><u>1,1</u>
NOW PROCESSING REGION:
                         1
OINITIAL MESH DEFINED USING THIS SCHEME:
    M
USE CURRENT SCHEME TO BEGIN PROCESSING? y
 GENERAL RECTANGLE PRIMITIVE PROCESSING USED
 -----
FURTHER PROCESSING STEPS: yes
 WF SMOOTHING PARAMETER FOR ISOPARAMETIC SET TO: 0.800
         1 SUCCESSFULLY COMPLETED AND SAVED
 REGTON
```

PROCESS ADDITIONAL REGIONS? no NUMBERING OF GENERATED OUTPUT BEGUN MESH PROCESSING COMPLETED

\*\* NODES: 9; ELEMENTS: 4; MATERIALS: 1 \*\* 

ENTER MESH OPTION:

ENTER OPTION: k,b

You will note that we processed this mesh stepwise, which in this case was a single step since the mesh contained just one region. The mesh scheme  $\mathbf{M}$  entered above is for a mapped mesh. You could have entered  $\mathbf{x}$  for a paved mesh. We will practice this in the tutorial session.

To actually view the mesh, just enter the graphics mode under the mesh layer to plot up the mesh.

g, p

\*\*

FASTQ is in one of two graphics sublayers; as you recall there is one under the top layer for viewing the geometry.

Now you need to add boundary information so Goma will know how to access the boundaries to apply boundary conditions. We will put in both node set and side set information from the b\*oundary section under the "keyin" mode. The difference between these will be explained in the Goma tutorials below.

From the mesh graphics level, enter , , k, b or enter 'return" twice and follow the text below.

THE FOLLOWING BOUNDARY FLAGS ARE AVAILABLE: P\*OINT FLAGS - FOR NODES AT POINTS N\*ODE FLAGS - FOR NODES ON A BOUNDARY E\*LEMENT FLAGS - FOR ELEMENT SIDES ON A BOUNDARY WHICH BOUNDARY FLAG WOULD YOU LIKE TO ENTER:

Enter "n" first and the following appears on your screen:

INPUT NODE BOUNDARY FLAG DATA IN THE FOLLOWING FORMAT: [ FLAG NO., LINE (OR NEG. SIDE) 1, LINE (OR NEG. SIDE) 2, ...] HIT RETURN TO END INPUT >1,1 >2,2 >3,3 >4,4 >

Now enter **b**, **e** to get to the input of side sets:

```
b,e
INPUT ELEMENT BOUNDARY FLAG DATA IN THE FOLLOWING FORMAT:
  [ FLAG NO., LINE (OR NEG. SIDE) 1, LINE (OR NEG. SIDE) 2, ...]
HIT RETURN TO END INPUT
>1,1
>2,2
>3,3
>4,4
>
```

What you have done here is define boundary flags 1-4 for both node sets and side sets. We will discuss how these flags will be used in the Goma tutorial below.

4. Now you need to re-generate the mesh (with the boundary flag info) and write out an EXODUS file. First, hit a few "returns" to get back to the top level, and then process the mesh. This time we will make it a 9-node element with an optimized node order; enter, m,ni,op,p,g,p for

```
m*esh, ni*ne, op*timize, p*rocess
g*raphics, p*plot (to look at the mesh)
```

Within the graphics subroutine you can toggle the display of many other quantities, like the node sets and side sets:

eb, nb, p\*lot

This toggles both the element boundary side sets and the nodal boundary side sets. You can zoom on the mesh by typing "z c" or "zoom cursor" and pointing and clicking to define the zoom area.

5. Now we are ready to write out the mesh. To do this you need to go up to the mesh level by hitting a return (or preceeding the write command with a comma, i.e., ,w). You should see the prompt ENTER MESH OPTION:

at which point you enter "w" for write and follow it by an EXODUS file name:

```
ENTER MESH OPTION: w
GENESIS DATABASE OUTPUT FILE NAME: box.exo
```

Note that we choose "box.exo" for the EXODUS file name.

6. Finally we need to make sure we save the mesh journal file, so that we can generate it again without all of these steps. To do this return to the root level with a "return" so you see **ENTER OPTION**:

Type in "write" or "w" and provide a name for the fastq file. We often use a ".fas" name extension to indicate that this is a fastq input file:

```
ENTER OPTION: w
FASTQ DATA FILE: box.fas
Now exit
```

ENTER OPTION: exit

7. Now for practice let us look at the mesh input file, box.fas:

more box.	fas						
TITLE							
POINT	1	0.0	000000	E+00	0.	0000	000E+00
POINT	2	1.0	000000	E+00	Ο.	0000	000E+00
POINT	3	1.0	000000	E+00	1.	0000	000E+00
POINT	4	0.0	000000	E+00	1.	0000	000E+00
LINE	1	STR	1	2	0	2	1.0000
LINE	2	STR	2	3	0	2	1.0000
LINE	3	STR	3	4	0	2	1.0000
LINE	4	STR	4	1	0	2	1.0000
REGION	1	1	-1	-2	-3	-4	
SCHEME	1 M	ye					
SCHEME	0 М						
BODY	1						
NODEBC	1	1					
NODEBC	2	2					
NODEBC	3	3					
NODEBC	4	4					
ELEMBC	1	1					
ELEMBC	2	2					
ELEMBC	3	3					
ELEMBC	4	4					
RENUM							
NINE							
EXIT							

Notice that all of your commands were journaled in this file. To regenerate the mesh just type fastq box.fas

```
_____
| Engineering Analysis Access Procedure for: fastq
| $Revision: 1.93 $, $Date: 1996/06/04 22:08:33 $
_____
Input options: -- box.fas
WELCOME TO FASTQ:
          DATE: 03/05/97
          TIME: 15:58:51
        VERSION: FASTQ 2.3X
+++
            Copyright 1988 Sandia Corporation
                                                 +++
+++ The U.S. Government retains a limited license in this +++
      software as prescribed in AL 88-1 and AL 91-7.
                                                 +++
+++
+++ Export of this program may require a license from the +++
               United States Government
+++
                                                 +++
FILE SUCCESSFULLY READ
TITLE:
  NUMBER OF POINTS READ:
                     4
```

```
NUMBER OF LINES READ:4NUMBER OF REGIONS READ:1NUMBER OF SCHEMES READ:1
```

ENTER OPTION:

From here just enter m, p, g, p to see the mesh followed by a , w to write it out.

For practice, edit the fastq file in the following way:

vi box.fas

to

Change the number of intervals on the lines to larger uneven numbers and the scheme to X for paving, i.e., change

LINE	1	STR	1	2	0	2 1.0000
LINE	2	STR	2	3	0	2 1.0000
LINE	3	STR	3	4	0	2 1.0000
LINE	4	STR	4	1	0	2 1.0000
REGION	1	1	-1	-2	-3	-4
SCHEME	1 M	iye				
SCHEME	0 М	I				
LINE	1	STR	1	2	0	<u>5</u> 1.0000
LINE	2	STR	2	3	0	7 1.0000
LINE	3	STR	3	4	0	<u>10</u> 1.0000
LINE	4	STR	4	1	0	<u>10</u> 1.0000
REGION	1	1	-1	-2	-3	-4
SCHEME	1 <u>x</u>	ye				
SCHEME	0 x					

Now regenerate the mesh with

fastq box.fas
m,p,g,p

Note how you now have an unstructured mesh in the same region.

Remember, the EXODUS file that is generated by fastq is in EXODUS I format. You must use **ex1ex2v2** to convert it to an EXODUS II format for use in Goma.

8. We will now take this box and extrude it into a square channel with GEN3D. This is actually simple and we encourage you to read the GEN3D manual to find out how to make more complicated shapes. Actually this only works with a 4-node quad being extruded into 8-node bricks, or hexes. So rerun fastq first and toggle the nine-node option (off) in the mesh generator and save the result in box.exo.

```
gen3d box.exo channel.exo
```

At the GEN3D prompt enter the following:

```
GEN3D> translate 10 5
```

and you will see

Translate mesh 10 times for a total of 5.000

Then to add on front and back node sets issue the following commands:

```
GEN3D> nset front 10
GEN3D> nset back 20
GEN3D> sset front 10
GEN3D> sset back 20
GEN3D> exit
```

Now to look at your results we will use BLOT, but the tutorial for BLOT is below, so we will show just basic commands here.

```
blot channel.exo
det
rotate x 45 y 45
p
nset
p
sset
p
```

These commands will pop an X window and show you the 3D mesh with the side and node sets.

- 9. GJOIN is a tool that can be used to join 2D and 3D meshes into larger meshes. Together with FASTQ and GEN3D some very complex meshes can be constructed. For now we will not demo GJOIN and refer you to the documentation, which has some nice examples.
- 10. GROPE can be used to extract and manipulate EXODUS I or EXODUS II files. Often times you want to extract a value of a variable at a specific location (node) or along a specific side (side set), like pressure along a permeable substrate, for instance. GROPE can be used to do this. The documentation is fairly complete and easy to understand.
- 11. ALGEBRA is similar to GROPE but allows you to define other variables based on your current nodal variable set. For instance, you may want to plot only dimensional quantities, even though your EXODUS file contains nondimensional ones. In ALGEBRA, you can define dimensional versions and output a new EXODUS file with those versions to be plotted by BLOT. Again, the documentation for ALGEBRA is complete and easy to understand.